Quantifying the topology of large–scale structure

Peter Coles, Andrew Davies & Russell C. Pearson,

Astronomy Unit, School of Mathematical Sciences, Queen Mary and Westfield College, Mile End Road, London E1 4NS

1 February 2008

ABSTRACT

We propose and investigate a new algorithm for quantifying the topological properties of cosmological density fluctuations. We first motivate this algorithm by drawing a formal distinction between two definitions of relevant topological characteristics, based on concepts, on the one hand, from differential topology and, on the other, from integral geometry. The former approach leads one to concentrate on properties of the contour surfaces which, in turn, leads to the algorithms CONTOUR2D and CONTOUR3D familiar to cosmologists. The other approach, which we adopt here, actually leads to much simpler algorithms in both two and three dimensions. (The 2D algorithm has already been introduced to the astronomical literature.) We discuss the 3D case in some detail and compare results obtained with it to analogous results using the CONTOUR3D algorithm.

Key words: Cosmology: theory – galaxies: clustering – large–scale structure of Universe – methods: statistical

1 INTRODUCTION

The recent dramatic increases in the quality and quantity of galaxy redshift data available to cosmologists, mapping larger and larger regions of our local Universe with increasing precision, has stimulated considerable interest in the development of sophisticated analysis techniques capable of extracting the essential characteristics of the spatial pattern displayed by such data. To get the most out of the current and next generation of redshift surveys requires techniques that can go beyond the traditional approach based on correlation functions (Peebles 1980). Only with appropriately specialised tools can such redshift data be used most effectively to constrain theoretical models of structure formation.

One approach towards characterising the properties of the large-scale distribution of matter in the Universe has been to measure objectively certain *topological* characteristics of the large-scale density field. This approach has generally involved the construction of contour surfaces of equal matter density. Then, with an appropriate algorithm, topological properties such as the *genus* (which quantifies the connectivity) of these surfaces can be calculated and compared with theoretical calculations or N–body simulations. This idea has led to a number of detailed analyses of both three–dimensional data (Gott, Melott & Dickinson 1986; Hamilton, Gott & Weinberg 1986; Weinberg, Gott & Melott 1987; Melott, Weinberg & Gott 1988; Gott et. al. 1989; Melott 1990) and angular (projected) distributions (Melott et al. 1989; Gott et al. 1992). A good review of this kind of analysis can be found in Melott (1990), where FORTRAN implementations of the algorithms normally used (i.e. CONTOUR2D & CONTOUR3D) are also given.

A particular advantage of the "genus" statistic, as it has come to be known, is that the mean value of this quantity can be calculated exactly for a Gaussian random field (Doroshkevich 1970; Adler 1981; Bardeen et al. 1986; Tomita 1986), the generic assumption for the initial density field in gravitational instability models. The behaviour of the genus can therefore be used to constrain the possibilities for non–Gaussian initial fluctuations using observations of galaxy clustering. The availability of the mathematical machinery to derive topological characteristics exactly for random density fields is another one of the motivations for using these characteristics as statistical descriptors.

In this paper we shall examine the "topological" approach from a mathematical point of view. We shall show that there are two distinct routes leading to technically different definitions of the relevant topological characteristics but that, in situations of relevance to cosmology, both the characteristics one derives are numerically equivalent or, at least, nearly so. The first route, based on a branch of mathematics known as differential topology, provides an elegant route to the derivation of the analytical results mentioned in the previous paragraph, through properties of the spatial derivatives of the contour surfaces.

The algorithms CONTOUR2D and CONTOUR3D, which are fairly complex, are also based on this line of thought. The second approach is based on a different mathematical foundation, provided by integral geometry (IG) rather than differential topology (DT). Unlike the first, it does not facilitate the elegant derivation of analytic results for Gaussian random fields. On the other hand, it does lead to algorithms for extracting topological descriptors from a given data set which are far simpler than those emerging from the former route.

Our approach is first to outline (briefly) these two mathematical approaches and explain how they lead to computations of essentially the same characteristics, but by very different routes. We then explain an algorithm based on the IG approach and show that it gives results which are indistinguishable from those obtained using CONTOUR3D, but which are obtained at a fraction of the computational cost. Those readers not interested in the mathematical niceties can skip directly to Section 3, where we describe our proposed algorithm and show the results of a test.

2   TECHNICALITIES

We shall be discussing the properties of *excursion sets* of a random field, $X(\mathbf{r})$, defined on an n–dimensional space, which we assume to be equipped with a Cartesian coordinate system made up of the unit vectors $\mathbf{e}_1, \ldots, \mathbf{e}_n$, so that $\mathbf{r} \in \Re^n$. The excursion set of X, called $\mathcal{A}_u$ is that subset of the space where X exceeds some specific level, say u. In general, the excursion sets of a random field may consist of many disjoint pieces, each of which may be simply or multiply connected. In cosmological applications, X is usually the density contrast $X = \delta \equiv (\rho - \rho_0)/\rho_0$, where ρ_0 is the mean matter density; δ has zero mean and, we assume, variance σ^2.

In practical situations the cosmological mass distribution is sampled, discretely, by some form of cosmic object (optical galaxy, infra-red galaxy, cluster of galaxies, etc.). In an N–body experiment, one is similarly hampered by discreteness effects. In order to construct the random field $X(\mathbf{r})$ one therefore needs to smooth the discrete distribution by convolving with an appropriate filter (Melott & Dominik 1993). Normally, this is done so as the produce a field defined on a Cartesian lattice, the most convenient representation for the forthcoming analysis.

We also have to consider the possibility that the excursion set may have an external boundary imposed upon it. For any particular sample, this will be determined by the edge of the survey region. In a simulation, the boundary may be the edges of the (usually cubic) region that is being simulated. Alternatively, in the second case, one can adopt periodic boundary conditions which dispense with the need for such considerations: here the space will be finite but will have no boundary. We shall touch on these considerations later.

The mathematical literature describes two distinct approaches towards characterising the topological properties of such sets. For elementary background material on related subjects, see Nash & Sen (1983). Much of the material presented here can be found in more rigorous fashion in Adler (1981).

2.1   Differential Topology

The first approach we shall discuss here employs concepts from the field of differential topology. We describe this approach first, as it is the more familiar in the astronomical literature. Essentially, one concentrates on properties of the bounding surfaces of the excursion set $\partial \mathcal{A}_u$ rather than on the set itself. Specifically, one relates topological properties of the excursion set to properties connected with the curvature of the surfaces bounding this set. This requires at the outset a number of non–trivial technical conditions to hold, relating to differentiability of these surfaces, which we shall not discuss here; see Adler (1981) for a technical discussion.

We start in a general way by considering a generic two–dimensional manifold $\mathcal{M}$, with a (one–dimensional) boundary $\partial \mathcal{M}$, which is piecewise smooth (i.e. it may have vertices where it is not differentiable). The general form of the Gauss–Bonnet theorem states that

$$\sum_{i=1}^{n} (\pi - \alpha_i) + \int_{\partial \mathcal{M}} k_g ds + \int_{\mathcal{M}} k dA = 2\pi \chi_E(\mathcal{M}), \tag{1}$$

where $\alpha_i, \ldots \alpha_n$ are the n interior angles of the vertices of the boundary $\partial \mathcal{M}$, k_g is the geodesic curvature of the curve $\partial \mathcal{M}$, and k is the ordinary (Gaussian) curvature of the manifold $\mathcal{M}$; ds and dA are elements of length and area respectively. The quantity χ_E is called the Euler, or Euler–Poincaré, characteristic of the manifold.

The case where there are vertices in the boundary is not particularly relevant in cosmology, so we shall drop this possibility from now on. The theorem (1) is relevant to the topology of both two– and three–dimensional excursion sets. First consider a two dimensional excursion set defined on a flat plane. Here the Gaussian curvature is everywhere zero and the Euler characteristic is simply given by an integral of the line curvature around the boundaries of the excursion set:

$$2\pi \chi_E = \int k_g ds. \tag{2}$$

In two dimensions, χ_E is simply the number of isolated regions minus the number of holes in such regions.

On the other hand, if we have a three–dimensional excursion set bounded by a two–dimensional surface which itself has no boundary: (e.g. a sphere, torus, etc) then the Euler characteristic is simply the integral of the Gaussian curvature of the surface over all compact pieces of the excursion set:

$$2\pi\chi_E = \int kdA. \tag{3}$$

In the three–dimensional case it has become fashionable to refer instead to the *genus*, g, an alternative topological quantity which is, roughly speaking, defined as the number of "handles" a compact two–dimensional surface possesses. A sphere has zero genus, a torus has unit genus, and so on. It is straightforward to show (Nash & Sen 1983) that

$$\chi_E = 2(1 - g). \tag{4}$$

The genus applies to three–dimensional sets (with two–dimensional surfaces) and has no direct equivalent in the case of two–dimensional sets (with one–dimensional "surfaces"); the Euler characteristic is, however, equally well–defined in both cases.

Notice that the genus (defined in this way) is not an additive characteristic. One can see this by taking the case of a set made up of two disjoint spheres. Each of these has genus zero so one would imagine the total genus of the set to be zero. On the other hand, the integrated curvature around each sphere must be 4π so the total for the set is 8π. The Gauss–Bonnet theorem (3) then tells us that $\chi_E = 2$ for each sphere and therefore the total $\chi_E = 4$. Straightforwardly applying eq. (4) then suggests $g = -1$ for this set. For the reason, and for technical reasons connected with sets which intersect boundaries (see Sec. 3 below), the practical implementation of the "genus statistic" in CONTOUR3D in fact does not employ the genus itself, but defines a quantity

$$g_S = -\chi_E/2, \tag{5}$$

which is additive. It is g_S rather than g as defined by equation (4) which is termed the "genus" in most of the cosmological literature.

One of the advantages of this approach is that one can relate the integrated curvature over a surface to the properties of the (discrete) set of critical points of that surface. The relevant branch of mathematics is known as Morse theory (Morse & Cairns 1969) and, using it, one can show, for example, that

$$\chi_E = \text{number of maxima} + \text{number of minima} - \text{number of saddle points}, \tag{6}$$

which is actually used by Bardeen et al. (1986) as the definition of the Euler characteristic. This equation, and/or eq. (3), allows one to relate global characteristics of each piece of the excursion set to local properties of the surface bounding it.

It is particularly relevant to note that one can exploit the properties of surface curvature to obtain the mean value of the Euler characteristic per unit volume (or area in 2D) for any random field X for which one has has the joint probability distribution of X and its first two spatial derivatives. In particular this can be accomplished for a Gaussian random field (Doroshkevich 1970; Bardeen et al. 1986; Hamilton et al. 1986; Tomita 1986). In fact, the Doroshkevich (1970) result predates the first derivations of this result in the mathematical literature (Adler 1976; Adler & Hasofer 1976; see also Adler 1981). Some special cases of non–Gaussian fluctuation fields are discussed in Coles (1988). For the particular case of relevance here, that of a Gaussian random field in three dimensions, it can be shown that

$$\chi_E(\nu) = A\left(1 - \nu^2\right)\exp\left(-\nu^2/2\right), \tag{7}$$

where the argument ν in equation (7) is the threshold density contrast, δ_t, defining the excursion set, expressed in dimensionless form: $\delta_t = \nu\sigma$, where σ is the rms value of δ. The quantity A, which is negative, simply depends on the *coherence length* of the field which, in turn, depends only on its power spectrum, so that all Gaussian random fields have a graph of $\chi_E(\nu)$ which has the same shape but an amplitude which depends on the initial power spectrum. (Recall that the power spectrum or, equivalently, the two–point correlation function, furnishes a complete description of the statistical properties of a Gaussian random field). Notice that χ_E is negative for $\nu = 0$, indicating multiple connectivity ($g > 1$): this is the so–called "sponge" topology (Gott, Melott & Dickinson 1986). At larger values of $|\nu|$, the topology approaches that of simply connected isolated regions (or holes) which become rarer and rarer as $|\nu|$ increases. As first pointed out by Doroshkevich (1970), the value of χ_E per unit volume for large ν leads to a useful approximation to the number density of local maxima, since each piece of the excursion set at high thresholds tends to consist of one isolated simply connected region containing one local maximum of δ. This situation, of isolated high-density islands surrounded by a low-density 'sea' is usually called a "meatball" topology while the opposite, low density regions embedded in a high-density background is, topologically speaking, equivalent to "Swiss–cheese".

The equation (3) can also used as a basis for extracting a measurement of χ_E from a given realisation of δ, estimated by smoothing galaxy data or particles in an N–body experiment. Here one must find some way of estimating the derivatives

of the contour surface, for example by fitting some form of polyhedral surface to it (Hamilton, Gott & Weinberg 1986). The algorithms CONTOUR2D and CONTOUR3D, written by D. Weinberg, are implementations of this idea; FORTRAN listings of these programs are available in Melott (1990).

2.2   Integral Geometry

The other approach, which is actually the older one historically speaking, uses the formalism of integral geometry (Hadwiger 1959; Adler & Hasofer 1976; Adler 1981). In this approach, one considers the excursion set to be constructed from objects known as *basic* sets. Let us define a k–dimensional hyperplane $\mathcal{E}$ to be a subset of $\Re^n$ such that any $(n-k)$ of the coordinates r_i are fixed; it is thus generated by k of the vectors $\mathbf{e}_1 \ldots \mathbf{e}_n$. A compact set $\mathcal{B} \subset \Re^n$ is a basic if the intersections of $\mathcal{B}$ with all possible k–dimensional hyperplanes are simply connected (including the case with $k = n$). One then takes the excursion set $\mathcal{A}$ (within a finite region of space) to be represented as the union of a finite number m of basics in such a way that the intersection of any of these basics is itself a basic; the formal proof that this can be done exists, but is not trivial (Adler 1981). Given this geometrical structure, one can then construct the Hadwiger characteristic $\phi_H(\mathcal{A})$:

$$\phi_H(\mathcal{A}) \equiv \underbrace{\sum \epsilon(\mathcal{B}_i)}_{(1)} - \underbrace{\sum \epsilon(\mathcal{B}_{i_1} \cap \mathcal{B}_{i_2})}_{(2)} + \cdots + (-1)^r \underbrace{\sum \epsilon(\mathcal{B}_{i_1} \cap \mathcal{B}_{i_2} \cdots \cap \mathcal{B}_{i_r})}_{(r)} + (-1)^m \epsilon(\mathcal{B}_{i_1} \cap \mathcal{B}_{i_2} \cdots \cap \mathcal{B}_{i_m}), \tag{8}$$

where $\sum_{(r)}$ means a sum over all combinations of $(i_1, \ldots, i_r)$ from the elements $(1, \ldots, r)$ and $1 \le r \le m$; $\epsilon(\mathcal{B})$ is the indicator function which is zero if $\mathcal{B}$ is the null set and equal to unity otherwise. This functional is, in fact, one of the Minkowski functionals (Mecke, Buchert & Wagner 1994); it possesses properties of invariance under translations and rotations, does not depend on how the set is partitioned into basics and also has the important property of additivity:

$$\phi_H(\mathcal{A}) + \phi_H(\mathcal{B}) = \phi_H(\mathcal{A} \cap \mathcal{B}) + \phi_H(\mathcal{A} \cup \mathcal{B}). \tag{9}$$

The summation (8) looks quite complicated, but can be shown to be equivalent to the following recursive (and much simpler) definition:

$$\phi_H(\mathcal{A}) = \text{number of disjoint intervals in } \mathcal{A} \qquad (n = 1) \tag{10}$$

and

$$\phi_H(\mathcal{A}) = \sum \left\{ \phi_H(\mathcal{A} \cap \mathcal{E}_x) - \phi_H(\mathcal{A} \cap \mathcal{E}_{x_-}) \right\} \qquad (n \ge 2), \tag{11}$$

where

$$\phi_H \left(\mathcal{A} \cap \mathcal{E}_{x_-} \right) = \lim_{y \to 0} \phi_H \left(\mathcal{A} \cap \mathcal{E}_{x-y} \right) \tag{12}$$

and the summation in (11) is taken over real x where the summand is non–zero. Note that the disjoint intervals counted in the one–dimensional case can be degenerate (i.e. points). This gives a very simple recursive algorithm for measuring the Hadwiger characteristic of the set, particularly in two dimensions as illustrated in Figure 1. In this case, the only allowed hyperplanes are lines. One simply scans a line parallel to the x-axis upwards through increasing values of y, noting the contribution to ϕ_H every time the number of intervals in the intersection of the line with $\mathcal{A}$ changes. The appropriate sum is then

$$\phi_H = \sum_x [N(x) - N(x_-)] = \sum_j C_j, \tag{13}$$

where $N(x)$ is the number of disjoint closed intervals, $N(x_-)$ is the relevant limit in eq. (12), and the sum is over a finite number of contributions C_j. Figure 1 shows how this works for a simply–connected set and for one with a hole in the middle. These figures are self–explanatory as long as one remembers to calculate the contributions C_j using the one–side limit (12) and that new intervals may be degenerate, i.e. they may appear first as points as one scans the line upwards. The application of this technique in three dimensions is more difficult to visualise, but is quite simple to program on a computer: one scans upward through the 3D excursion set, slicing it using 2D planes, and scans each plane with 1D lines in the manner described previously.

We have tacitly assumed so far that the excursion set does not intersect any external boundary $\mathcal{C}$. Of course, the question of edge effects does not arise if one is dealing with periodic boundaries, such as in typical N–body simulations. In calculating the DG characteristics with CONTOUR3D, for example, one simply allows the algorithm to 'wrap-around' the edges of the simulation box.

Correction for boundary effects is slightly less straightforward in the context of the IG characteristic. If we are dealing with a simulation box, one can allow the IG algorithm to wrap-around as in the case mentioned in the previous paragraph. This is, in fact, equivalent to subtracting off the characteristic of the set comprising the intersection $\mathcal{A} \cap \mathcal{C}$, where $\mathcal{C}$ is the coordinate boundary of the box (for a periodic simulation this is not really a physical boundary). For example, if one has an

Figure 1. The recursive calculation of the Hadwiger characteristic in two dimensional examples. The left figure shows a simply–connected set with $\phi_H = 1$, while the right figure has one region containing one hole: $\phi_H = 0$. The y-axis is labelled with the number of disjoint intervals and the values of C_j at the points where the value of $N(x)$ changes.

excursion set embedded in a cubic volume, one subtracts from the 3D characteristic the 2D characteristics generated by the intersection of the set with the three planes with the origin at one corner:

$$\chi_H = \phi_H(\mathcal{A}) - \phi_H(\mathcal{A} \cap \mathcal{C}_0), \tag{14}$$

where $\mathcal{C}_0$ indicates that part of the boundary which has the origin at a vertex. This formulation of the boundary correction is a straightforward consequence of the definition of ϕ_H given above, in equation (8). Notice, however, that there is a problem with this definition: in the case of sets which intersect the boundary, but do not have the same number of intersections with each part of the boundary, this procedure gives a different result depending on which of the coordinate axes one chooses as the x-axis in the above operation; see, for example, Figure (4.4.2) of Adler (1981). The differential geometry characteristic, on the other hand, is invariant with respect to transformations of the coordinate axes in this way. If we are going to use the IG approach as an estimator of χ_E, therefore, we are immediately restricted to sets which are effectively 'isotropic'. This effectively means that we must be dealing with a large enough sample of the random field that it contains regions oriented in all possible ways with respect to the coordinate axes. This is one aspect of the need to have a 'fair sample' of the Universe in order to estimate global characteristics from local samples. Notice that this is a stronger requirement than the requirement that the field be *ergodic*. The property of ergodicity is, roughly speaking, that spatial averages over an infinite domain are equivalent to averages performed over the probability distribution. For many statistical analysis tools, including the IG characteristic, to be useful one actually needs the average over a finite volume to produce a result within some acceptable range of the average of the distribution. Whether a given technique fulfills this particular criterion for 'usefulness' is a question that has to be answered on an individual basis. Ergodicity would appear to be a necessary condition for usefulness, but not in all cases a sufficient one.

   Adler (1981) advocates χ_H (he calls it Γ) as the most appropriate definition of an IG-equivalent to the DG characteristic χ_E: an alternative, not equivalent to χ_H, has been suggested by Fava & Santalo (1979) which also attempts to take account of the lack of coordinate invariance of χ_H. Exact correction for boundary effects can be made using the complete set of Minkowski functionals (Likos et al. 1995; Schmalzing, Kerscher & Buchert 1996). Notice that χ_H only coincides with ϕ_H if there are no intersections of the set with the boundary. In addition, if the field is periodic then these two quantities coincide again: the boundary correction cancels as we mentioned above. If one has a cubic volume within a non-periodic field then adopting this boundary correction is tantamount to assuming the field is periodic outside the volume and this will introduce some error in χ_H as an estimator of χ_E. In a practical situation one would require the boundary correction to be small in this circumstance, otherwise one cannot claim to have a 'fair sample'.

Our discussion of boundary corrections has so far been restricted to the case of cubic boundaries. In reality, boundaries of galaxy surveys are likely to be much more complicated than this. There are two different ways to view this problem. First, one can try to implement a rigorously-defined boundary correction in order to produce an estimate from the sample which is as close as possible to the global average defined over the probability distribution. In this vein, Alder (1981, p. 78) gives a concise way of extending the boundary correction in equation (14) to more complicated shapes. Another possibility is to attempt to eliminate the boundary by a weighted averaging method (Coles 1988; Coles & Plionis 1991; Davies & Coles 1993; Davies 1994). On the other hand, a more pragmatic approach would suggest not worrying too much about the accuracy of the estimate of global quantities from finite samples, particularly if the boundary is complicated and the sample is small. If one is really interested in testing observations against model simulations constructed with the same boundaries and selection effects then, as long as one does the same correction for the data as is done for the models, the precision of the correction will not affect the robustness of the test. If the correction is large compared with the true signal, however, then such a test will have no power as differences between simulation and data will be masked by artificial noise introduced by an uncontrolled boundary correction. One would therefore hope that the samples used for any such test should be 'useful' in the sense defined above and this, in turn, requires that samples be large enough so as not to be dominated by boundary effects, whether the boundary be a simple cube or a more complicated shape, in much the same way as they need to be large in order not to be greatly affected by changes in orientation as discussed above. We shall discuss these practical issues further, in Section 3 below.

Notice that this definition does not require the construction of a continuous field on a lattice. One way of treating galaxy data, for example, is simply to "decorate" each galaxy with a sphere (a sphere is a basic) so that the excursion set is the union of such spheres. One can then study the behaviour of ϕ_H as a function of the radius of the sphere. This approach, which is reminiscent of that used in traditional percolation analysis (e.g. Zel'dovich, Einasto & Shandarin 1982), is described in detail in Mecke, Buchert & Wagner (1994) and Schmalzing et al. (1996), and also mentioned below.

On the other hand, one often has to deal with some discretised version of X, perhaps defined on a Cartesian lattice, and consequently one has a discretised version of the excursion set in which one cannot locate exactly in $\Re^3$ those points where $\phi_H(\mathcal{A} \cap \mathcal{E}_x)$ changes. This would appear to pose some technical problems. Fortunately, there is a straightforward implementation of this method to sets defined on regular lattices.

A two–dimensional implementation of this idea is found in Adler (1981); it was introduced to cosmology by Coles (1988) in the context of regions of high or low temperature on the microwave background sky, and is illustrated in Figure 2. The trick is simply to regard each "basic" making up the excursion set as being approximated by the lattice itself. In 2D, therefore, the basics are approximated as collections of squares, lines and points. In 3D, we have also cubes. By simply counting these components one can easily derive an approximation to the characteristic defined by equation (8), which is accurate as long as the lattice has a finer grid than the typical size of pieces of the excursion set. The formal proof is given in Adler (1981, p119); some practical issues are discussed in Davies (1994). If the excursion set is approximated as S squares, H horizontal lines, V vertical lines and P points then

$$\phi_H = S - [V + H] + P. \tag{15}$$

Points are counted regardless of whether they belong to lines or squares; lines are counted regardless of whether they belong to squares. More detailed investigations of the properties of this algorithm for two–dimensional galaxy clustering data are described elsewhere (e.g. Coles & Plionis 1991; Plionis, Valdarnini & Coles 1992; Davies & Coles 1993; Coles et al. 1993; Davies 1994).

Corrections for square boundaries can be calculated, where appropriate, by counting the number of points P^*, horizontal lines H^*, and vertical lines V^*, in the intersection of the excursion set with the x and y axes. One then obtains χ_H according to

$$\chi_H = \phi_H - [P^* - V^* - H^*]. \tag{16}$$

Methods for dealing with more complicated boundaries are discussed by Coles & Plionis (1991), Davies & Coles (1993) and Davies (1994).

We shall describe the analogous three–dimensional algorithm for lattice data in Section 3.

2.3   Comments

The Euler characterisic χ_E and the Hadwiger characteristic ϕ_H differ in that they are defined for different classes of sets and are handled with different kinds of mathematical machinery. In cases where these two classes overlap, however, the two definitions are in fact identical (apart from the treatment of boundaries). Since the sets in which we are interested actually belong to this overlapping class, we shall henceforth drop the subscripts and change the notation to refer to χ as the Euler–Poincaré characteristic, regardless of the way it is measured. The important point to be made here is that, although the differential topology approach of section 2.1 is clearly the more elegant route to a mathematical derivation of the mean value

Figure 2. The 2D "lattice" calculation of the Hadwiger characteristic. The points inside the contour lie above the threshold and those outside lie below. Orthogonal lines are drawn from each point above the threshold to neighbours which are also above the threshold. In this example the resulting network has 2 squares, 10 vertical lines, 12 horizontal lines and 21 points. The characteristic then takes the value $\chi = 2 - (10 + 12) + 21 = 1$, as expected.

of χ for the excursion sets of a Gaussian random field, that does not imply that this is necessarily the best way also to measure the value of χ for a given practical realisation of an excursion set. In fact, it should now be obvious that this is not the case: the slicing of a geometrical body with lines and planes involves much simpler mathematical concepts and is therefore much easier to implement on a computer than is the numerical differentiation of a fit to the surface of the body.

The algorithm presented in 2.2 gives a much simpler (and faster) way of extracting χ for a set of contour data than integrating the curvature of each contour line around each compact subset of $\mathcal{A}_u$. As we shall see, three–dimensional analyses are simplified even further by the IG approach. As a practical measuring tool, therefore, the 3D version of the IG (Hadwiger) characteristic is generally to be preferred.

3 THE 3D IG ALGORITHM

It is first worth re-iterating the point we made above that the IG approach does not require data to be presented on a lattice. It is possible to surround each "galaxy" in a sample by an appropriately–chosen basic (e.g. a sphere), and then proceed to slice it in one and two dimensions according to the prescription of Sec 2.2. This approach has been elaborated by Mecke, Buchert & Wagner (1994) and Schmalzing et al. (1996), so we will not discuss it further, though it is an additional clear advantage of the IG approach.

The "lattice" algorithm for 3D data is a straightforward generalisation of the 2D version described above, and is given mathematical motivation by Adler (1981, p. 121). In this case, one approximates the shape of the 3D excursion regions by connecting points above the threshold into a network of C cubes, S squares, V vertical lines, H horizontal lines and P points. Points, squares and lines are counted whether or not they belong to cubes, and so on, in an analogous manner to the 2D definition. The appropriate approximation to the Euler–Poincaré characteristic is then just

$$\chi = \phi_H = -C + S - [V + H] + P \tag{17}$$

(Adler 1981). Once again, one has to be a little careful about boundaries. If there is a simple cubic boundary and one either has a periodic simulation or is prepared to assume the correction regardless, then one simply uses the correction described in Sec. 2.2, namely to subtract off the 2D characteristic of the intersection of the excursion set with the boundary edges evaluated using the 2D algorithm. As pointed out above, this means evaluating three 2D characteristics, one for each of the

three faces of the cube which contain the origin. One can estimate the error in this correction by simply choosing the origin to be at different corners of the cube. If these faces contain P^* points, V^* vertical lines, H^* horizontal lines and S^* squares, then

$$\chi' = \chi_H = \chi - (S^* - [V^* + H^*] + P^*), \tag{18}$$

where the prime indicates that a boundary-corrected quantity is being used. The definition (18) is particularly convenient for simulation data which are usually presented on such a periodic lattice.

If the boundaries are more complicated than this, such as is almost certainly the case with a real galaxy sample, then one has to work a little harder. One approach is one discussed by Coles & Plionis (1991), Davies & Coles (1993) and Davies (1994): one simply takes a weighted average the characteristic of the excursion set with that of the complementary set, i.e. the sample volume minus the excursion set; this could be called the *incursion set*. Since a connected region in the excursion set becomes a hole in the incursion set, the characteristics of these two sets should be equal (up to a sign), except for the region around the edge. This method works well in two-dimensions. In a separate paper (Pearson et al. 1996), we are applying the IG tool to the Abell/ACO cluster sample and simulations of it based on various models of cosmological structure formation. Even though this sample is relatively small and has a complex boundary, the correction is small compared to the realisation-to-realisation variance in the estimator (actually, about 10%).

It should be said again that the DT characteristic does not require any such boundary correction. Since the results of CONTOUR3D are usually expressed in terms of g_S, which is defined to be related to an integral of the curvature of the excursion set surfaces. When one reaches any boundary, therefore, one simply stops integrating. In practical situations, however, this difference is unimportant because, in order to be useful anyway, a sample should have a relatively large ratio of interior volume to external boundary.

Figure 3 shows a comparison of the results of the results obtained using our IG approach with analogous results obtained using CONTOUR3D (which, as we have explained, is a product of the DT formalism). For simplicity, we generated a single random-phase realisation of a Gaussian random fields with a white–noise power spectrum on a 64^3 grid and then analysed it with both algorithms. The simulations actually have periodic boundary conditions so we can implement the Adler (1981) correction in the IG case. We have not inserted error bars on these curves, so one can see the detailed behaviour of both algorithms more clearly. Notice that the departures from the Gaussian curve are similar for both algorithms: on the top simulation, with a smoothing length of 2.5 grid cells, the rms difference between the two different measurements of χ for this simulation is of order 0.07 in the units displayed on the y-axis. This is to be compared with a variation in χ from simulation to simulation of order 0.15 determined by performing an ensemble of simulations of this kind. This is consistent also with the visual estimate of the scatter around the ensemble mean. Note also that the difference between boundary–corrected and uncorrected IG estimates is of order 0.03 in this example, negligible compared to the ensemble variation. These errors are smaller when the smoothing is decreased because coherence length of the field then decreases so that the excursion set consists of more regions and the effects discussed previously in connection with the 'fair sample' requirement are strongly reduced. Notice that the coherence length of the field also determines the amplitude of the curve: we have scaled this out in these two examples.

Of course there are situations where the two methods might give results that diverge greatly from each other. If one had a very large ratio of coherence length to sample size or a very large grid spacing, then dealing with the boundary can pose problems and the method may be inaccurate. On the other hand, even this may not be too much of a problem in practice. Re-iterating a point we made in Section 2, one is almost always dealing with a comparison between simulated and observed data sets: if one is only interested in testing a particular model then it is less important that a statistic provides an unbiassed estimate of some globally defined quantity than that it provides a robust dicriminator between theory and observation. To a large extent, therefore, one really needs to ensure only that the same thing is done to both real and simulated data (same gridding procedure, same boundary, same smoothing, same correction, etc). A much more detailed investigation of a confrontation between model and theory using the IG method is discussed in Pearson et al. (1996).

One should be aware, however, that estimates of χ made using the IG method from a finite sample are not guaranteed to be unbiassed: one would have to check this carefully using an ensemble of simulations and adjust any corrections accordingly. This should warn against using our method to estimate the coefficient A in equation (7) unless the boundary correction were well–controlled. In any case, the quantity χ is not a very efficient estimator of A so one probably would not wish to employ either the IG or DT versions of the algorithm to estimate the coherence length (and hence the power spectrum) anyway. The topology of the QDOT survey yields only very weak constraints on the index of the power spectrum of galaxy clustering (Moore et al. 1992). The potential usefulness of χ lies in its capability to detect non–Gaussian behaviour whether it be primordial or induced by non-linear gravitational evolution of initially Gaussian density perturbations.

Figure 3. Comparison of the results obtained, as a function of ν_2, for the 3D lattice algorithm (left, labelled "EPC") and CONTOUR3D (right, labelled "GENUS"). The sign of the EPC curve has been changed to the y-axis scaled by a factor two as indicated by equation (5), in order to make the results directly comparable. The simulations used were of an uncorrelated (i.e. Poisson) Gaussian random field defined on a 64^3 grid, smoothed on two different length scales using a Gaussian filter. Results are virtually indistinguishable. Taken from Davies (1994).

4 DISCUSSION

In this paper we have introduced an alternative algorithm for quantifying the topology of excursion sets, with the aim of producing a simpler tool for measuring the connectivity properties of high and low density regions in cosmological density fields.

The approach we adopt differs in its mathematical motivation from the "traditional" approach. We have therefore gone to some length to attempt to explain the foundations of the different approaches to topological analyses based on differential topology (DT), on the one hand, and integral geometry (IG) on the other. The central point to emerge from these considerations is that the DT approach is better for handling the properties of random fields analytically (mainly because one can use the powerful mathematics of Morse theory to relate integrated curvature to the simple counting of critical points). The IG approach, although not conducive to analytic studies to anything like the same extent, nevertheless generates much simpler algorithms for measuring the relevant characteristics in practical situations. Importantly (though we did not include the proof here), the situations in which we are interested in exploiting such characteristics involve objects which can, in principle, be treated with either approach. The moral of this tale is, therefore, that DT is better for theory, IG better for practice.

Although the IG algorithm has the advantage of being faster (it is also parallelisable), this is probably not a particularly relevant consideration for present large–scale structure studies because the computation of the so–called "genus" curves is

not in any case an arduous task. Future generations of redshift surveys, which will be an order of magnitude larger in size than existing ones may invalidate this argument. Our particular motivation for favouring this algorithm at the present time, however, has been the need to analyse the topological properties of a huge ensemble of realisations of large–scale cluster simulations (Borgani et al. 1995), for which the speed and simplicity of the new algorithm has great advantages. This latter study, (Pearson et al., in preparation), which also takes into account percolation properties and measures of "filamentariness", is intended to provide a theoretical understanding of the differences in clustering pattern for models which differ only slightly in their initial power spectra and cosmological parameters. Quite apart from this specific argument, however, we stress the more obvious point that simpler algorithms should generally be preferred to complicated ones which produce the same results.

REFERENCES

Adler R.J., 1976, J. Appl. Prob., 13, 276
Adler R.J., 1981, The Geometry of Random Fields. John Wiley & Sons, New York
Adler R.J., Hasofer A.M., 1976, Ann. Prob., 4, 1
Bardeen J.M., Bond J.R., Kaiser N., Szalay A.S., 1986, ApJ, 304, 15
Borgani S., Plionis M., Coles P., Moscardini L., 1995, MNRAS, 277, 1191
Coles P., 1988, MNRAS, 234, 509
Coles P., Moscardini L., Plionis M., Lucchin F., Matarrese S., Messina A., 1993, MNRAS, 260, 572
Coles P., Plionis M., 1991, MNRAS, 250, 75
Davies A.G., 1994, Statistical Studies of Cosmological Density Fields. PhD Thesis, Queen Mary & Westfield College, University of London
Davies A.G., Coles P., 1993, MNRAS, 260, 553
Doroshkevich A.G., 1970, Astrofizika, 6, 320
Fava N.A., Santalo L.A., 1979, Z. Wahrscheinlichkeitstheorie verw. Gebiete, 50, 85 [in English]
Gott J.R. et al., 1989, ApJ, 340, 625
Gott J.R., Mao S., Park C., Lahav O., 1992, ApJ, 385, 26
Gott J.R., Melott A.L., Dickinson M., 1986, ApJ, 306, 341
Hadwiger H., 1959, Math. Z., 71, 124
Hamilton A.J.S., Gott J.R., Weinberg D.H., 1986, ApJ, 309, 1
Likos C.N., Mecke K.R., Wagner H., 1995, J. Chem. Phys., 102, 9350
Mecke K.R., Buchert T., Wagner H., 1994, A& A, 288, 697
Melott A.L., 1990, Physics Reports, 193, 1
Melott A.L., Cohen A.P., Hamilton A.J.S., Gott J.R., Weinberg D.H., 1989, ApJ, 345, 618
Melott A.L., Dominik K.G., 1993, ApJS, 86, 1
Melott A.L., Weinberg D.H., Gott J.R., 1988, ApJ, 328, 50
Moore B., Frenk C.S., Weinberg D.H., Saunders W., Lawrence A., Ellis R.S., Kaiser N., Efstathiou G., Rowan–Robinson M., 1992, MNRAS, 256, 477
Morse M., Cairns S., 1969, Critical Point Theory in Global Analysis and Differential Topology. Academic Press, New York
Nash C., Sen S., 1983, Topology and Geometry for Physicists. Academic Press, London
Peebles P.J.E., 1980, The Large–scale Structure of the Universe. Princeton University Press, Princeton
Plionis M., Valdarnini R., Coles P., 1992, MNRAS, 258, 114
Schmalzing J., Kerscher M., Buchert T., 1996, in Bonometto S., Primack J., Provenzale A., eds, Proceedings of International School 'Enrico Fermi' CXXXII, Dark Matter in the Universe, Institute of Physics, in press
Tomita H., 1986, Prog. Theor. Phys., 76, 952
Zel'dovich Ya. B., Einasto J., Shandarin S.F., 1982, Nat, 300, 407